# An Overture Overview

Bill Henshaw

Centre for Applied Scientific Computing,
Lawrence Livermore National Laboratory,
Livermore, CA, USA 94551

www.llnl.gov/casc/Overture

Presented at the Seventh DOE ACTS Collection Workshop, August 2006.



## Acknowledgments

### Supported by

Department of Energy, Office of Science
MICS Program: Mathematical, Information, and Computational Sciences
SciDAC: Scientific Discovery through Advanced Computing

### Current Overture developers

Kyle Chand
Bill Henshaw

### Collaborators

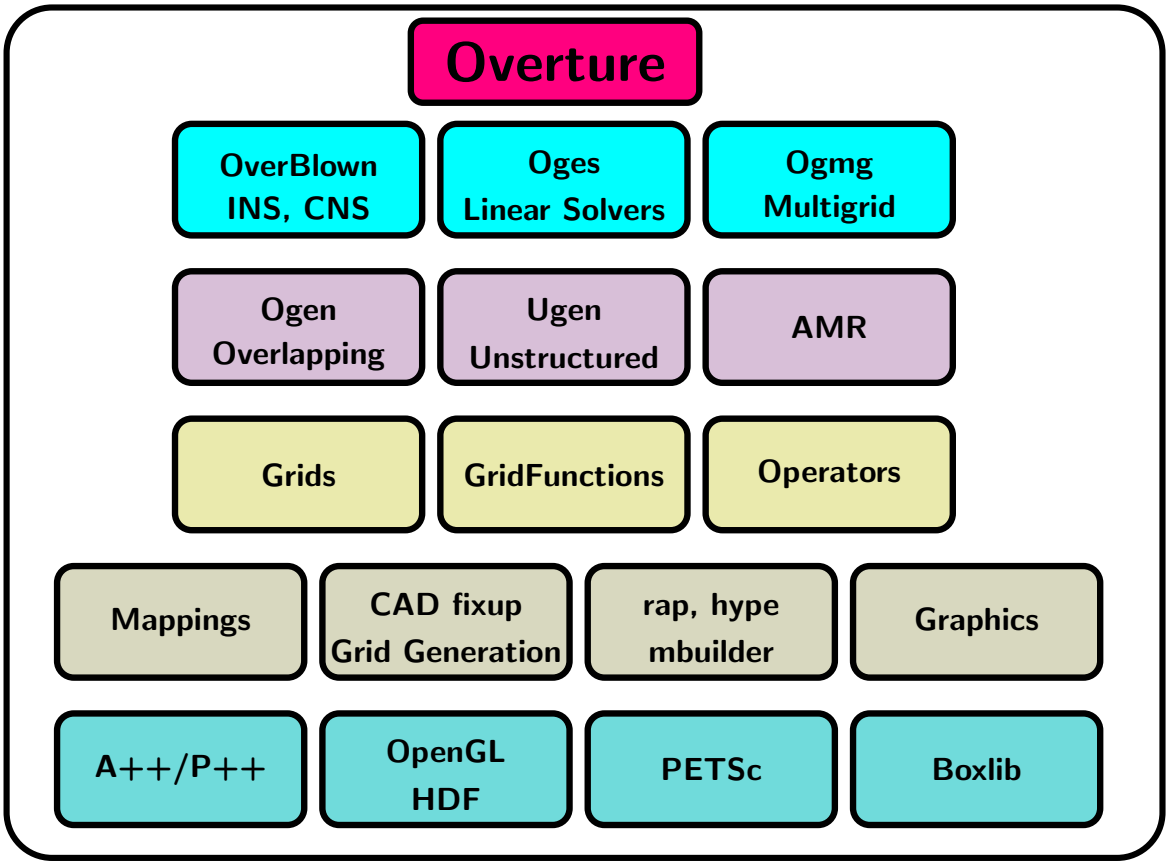
Don Schwendeman (RPI),
Tom Hagstrom (UNM),
Jeff Banks (SNL)
Nikos Nikiforakis (U. Cambridge),
Petri Fast (LLNL)

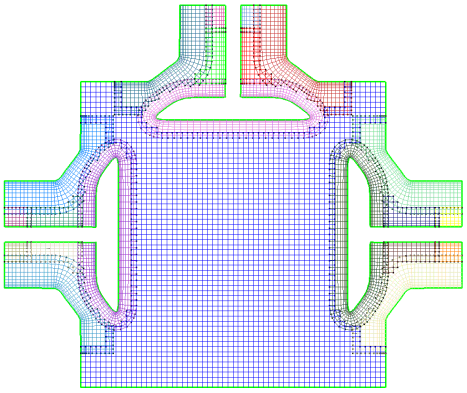
## Overture is a collection of C++ classes that can be used to solve partial differential equations on structured, overlapping and hybrid grids.

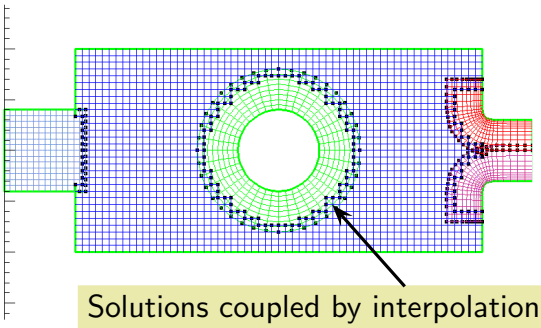
**Key features:**

- provides a high level interface for rapid prototyping of PDE solvers.
- built upon optimized C and fortran kernels.
- provides a library of finite-difference operators: conservative and non-conservative, 2nd, 4th, 6th and 8th order accurate approximations.
- support for moving grids
- support for block structured adaptive mesh refinement
- extensive grid generation capabilities
- CAD fixup tools
- interactive graphics and data base support.
- PDE solvers built upon Overture include:
  - OverBlown: incompressible Navier-Stokes, compressible Navier-Stokes, reactive Euler equations.
  - MX: time domain Maxwell's equations solver: fourth-order accurate, parallel.



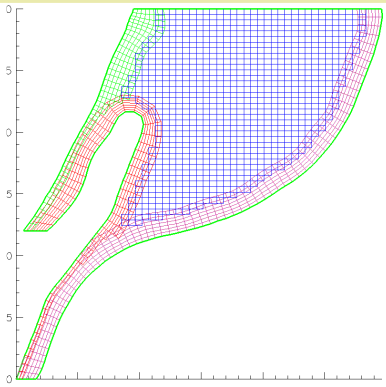


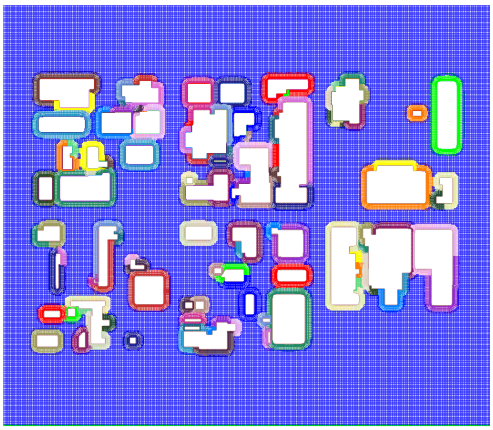




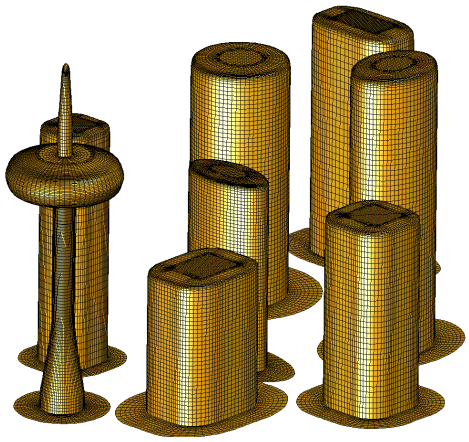
Solutions coupled by interpolation

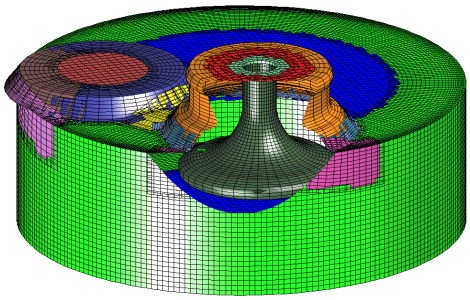
Sample 2D overlapping grids



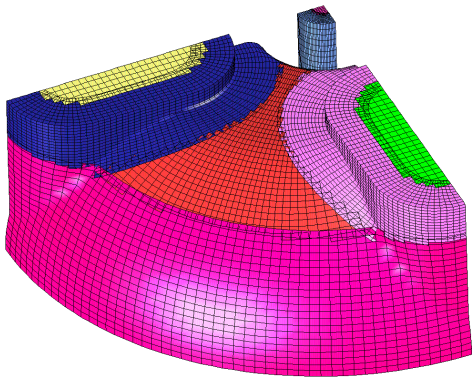


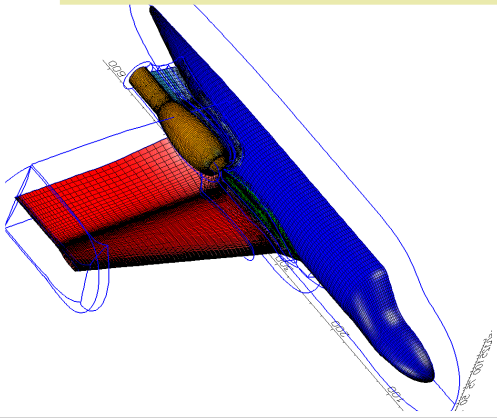
5





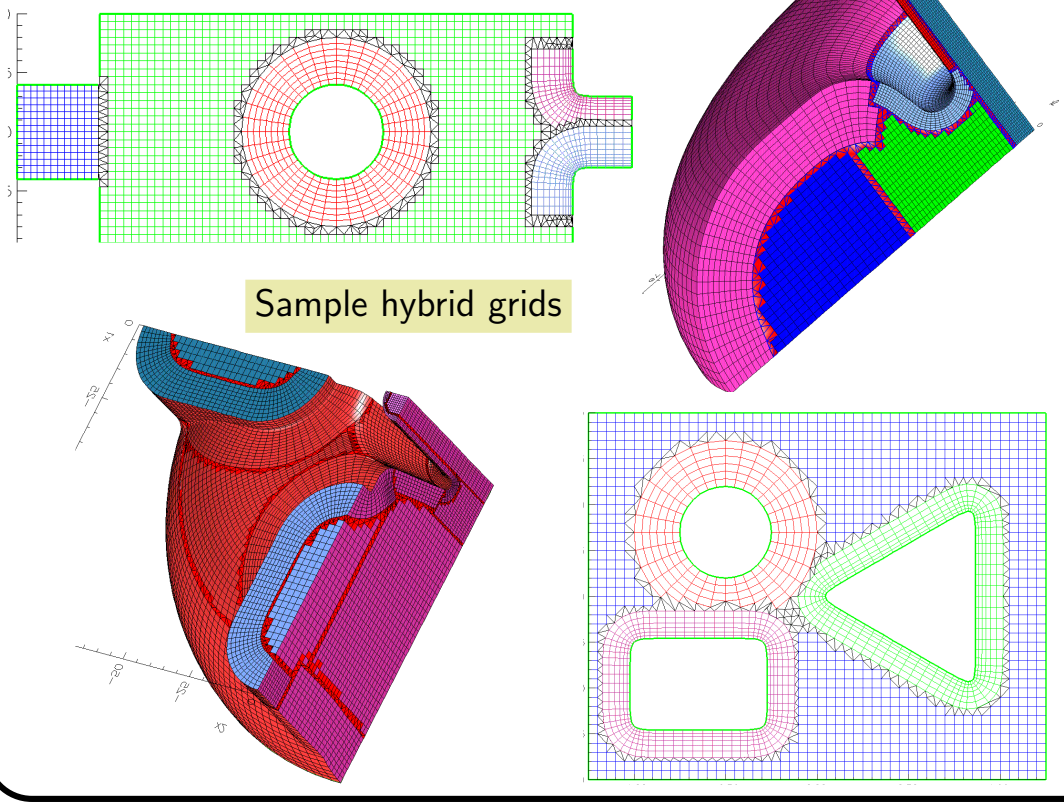
Sample 3D overlapping grids





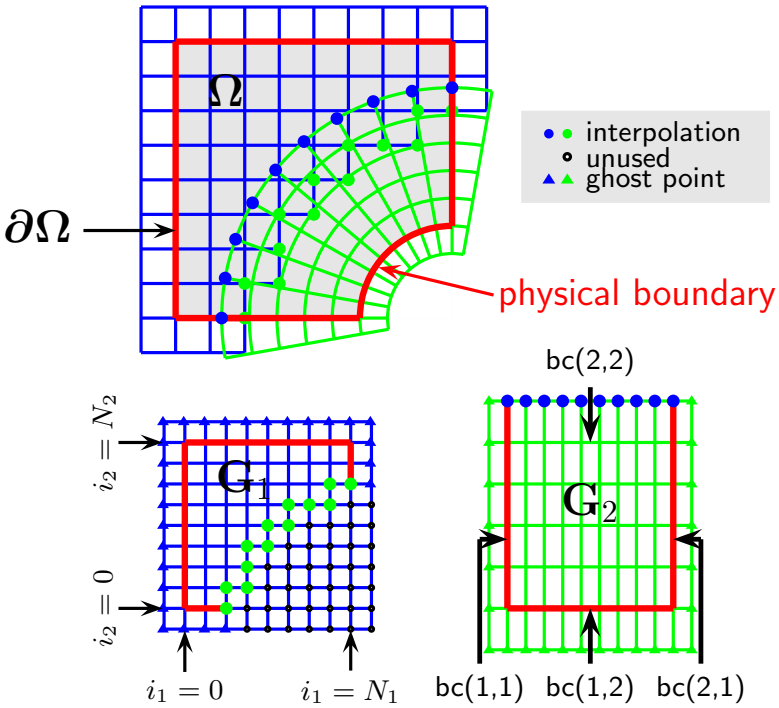
6

## Sample hybrid grids





## Components of an Overlapping Grid



## Overture supports a high-level C++ interface (but is built mainly upon Fortran kernels):

Solve $u_t + au_x + bu_y = \nu(u_{xx} + u_{yy})$

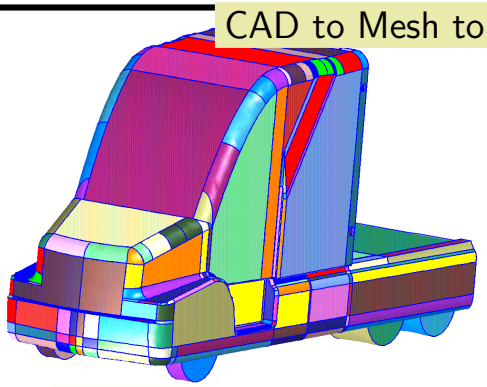
```
CompositeGrid cg;  // create a composite grid
getFromADataBaseFile(cg,"myGrid.hdf");
floatCompositeGridFunction u(cg);  // create a grid function
u=1.;
CompositeGridOperators op(cg);  // operators
u.setOperators(op);
float t=0, dt=.005, a=1., b=1., nu=.1;
for( int step=0; step<100; step++ )
{
  u+=dt*( -a*u.x()-b*u.y()+nu*(u.xx()+u.yy()) ); // forward Euler
  t+=dt;
  u.interpolate();
  u.applyBoundaryCondition(0,dirichlet,allBoundaries,0.);
  u.finishBoundaryConditions();
}
```



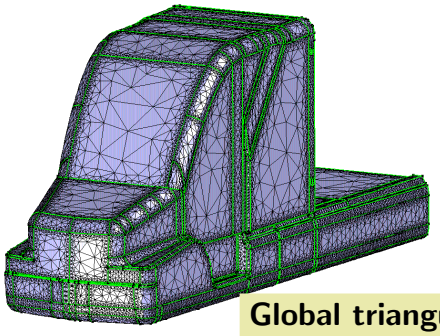
## Current Projects with Overture

- Support for multi-physics problems, for example:
  - incompressible fluid flow coupled to solid heat transfer
  - compressible fluid flow coupled to solid mechanics
- Electromagnetics, time dependent Maxwell's equations.
- High speed reactive flow with moving grids adaptive mesh refinement (Don Schwendeman (RPI))
- Compressible multiphase flows (Don Schwendeman (RPI))
- Compressible multi-material flows (Jeff Banks (SNL))
- Deforming boundaries in incompressible flow (Petri Fast)
- Compressible flow with ice formation (Graeme Leese).
- Einstein field equations (Philip Blakely)
- Hybrid (unstructured) grid algorithms (Kyle Chand)
- Compressible axisymmetric flow with swirl (Kyle Chand)

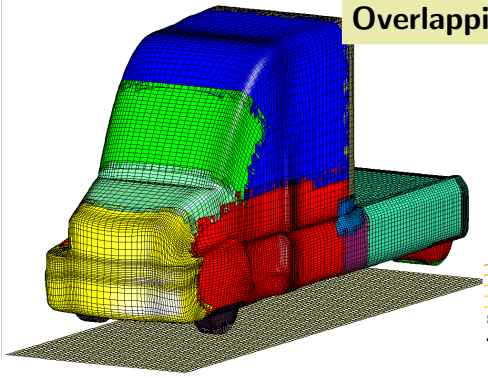
## CAD to Mesh to Solution with Overture



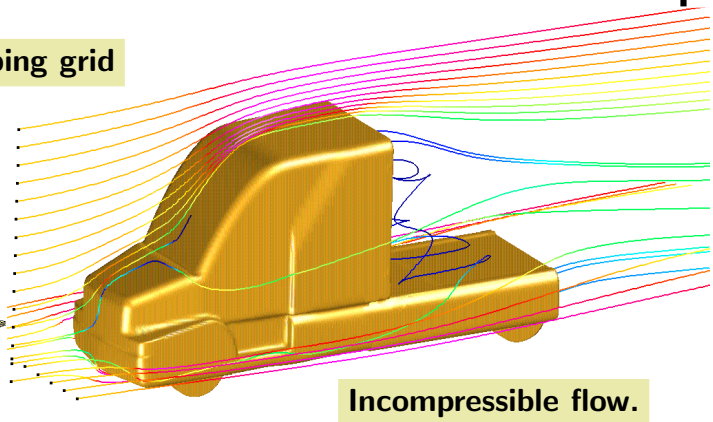
Cad fixup



Global triangulation



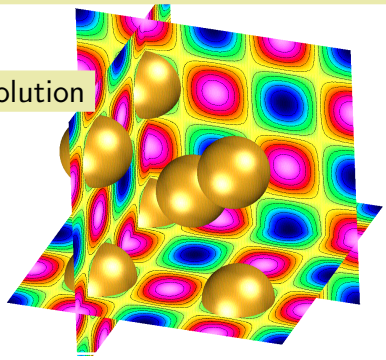
Overlapping grid



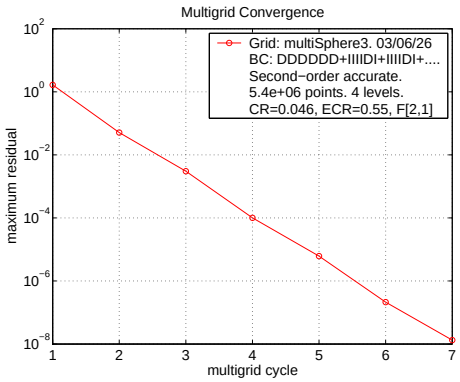
Incompressible flow.

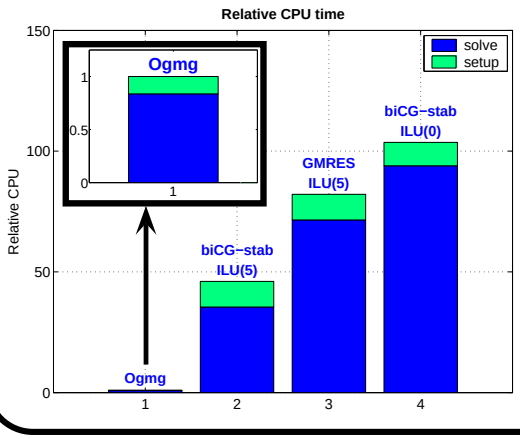


## Multigrid solution to Poisson's equation, 5.4 million grid points



solution

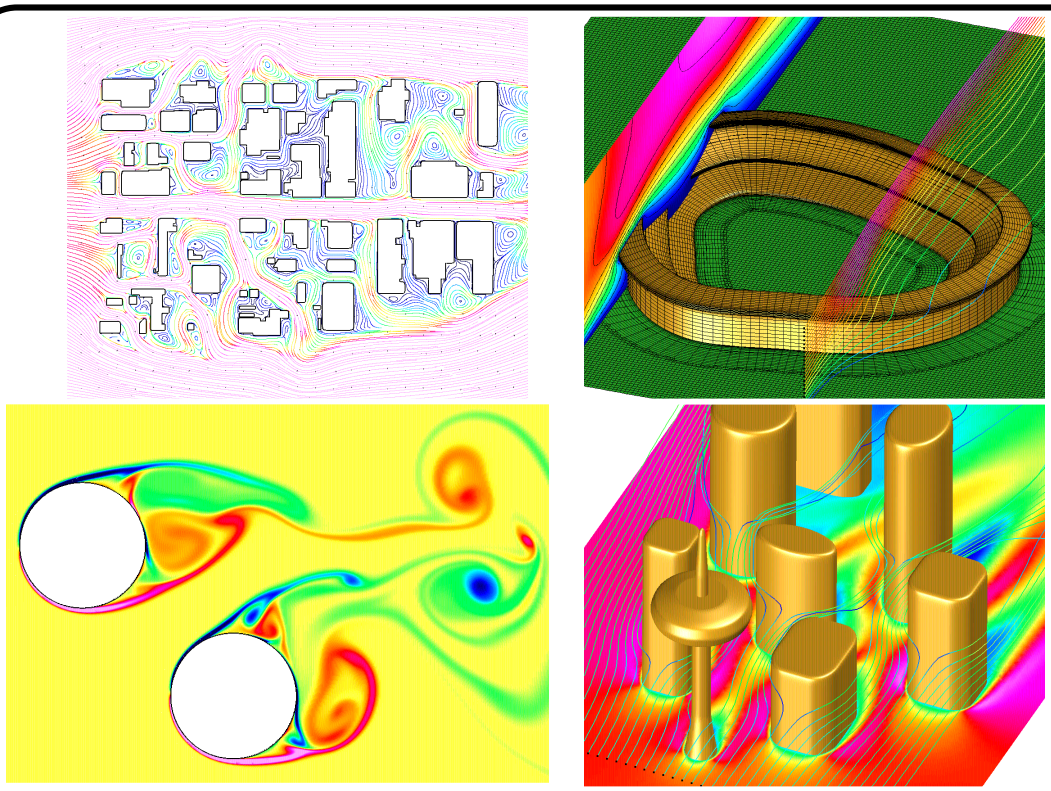



Mesh independent convergence rates

New adaptive MG for overlapping grids.

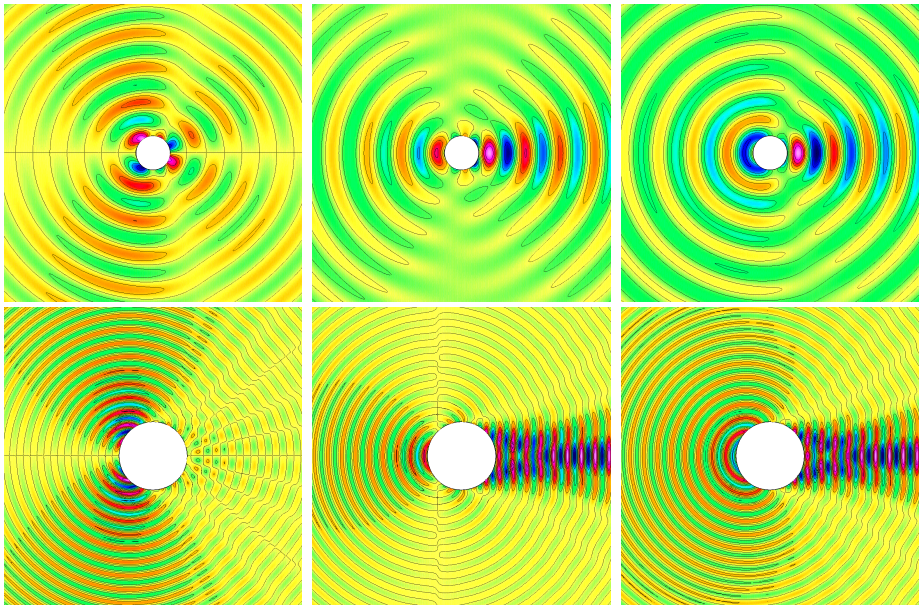
In comparison to Krylov solvers multigrid is an order of magnitude faster and uses an order of magnitude less storage



Incompressible flow computations with OverBlown.

13

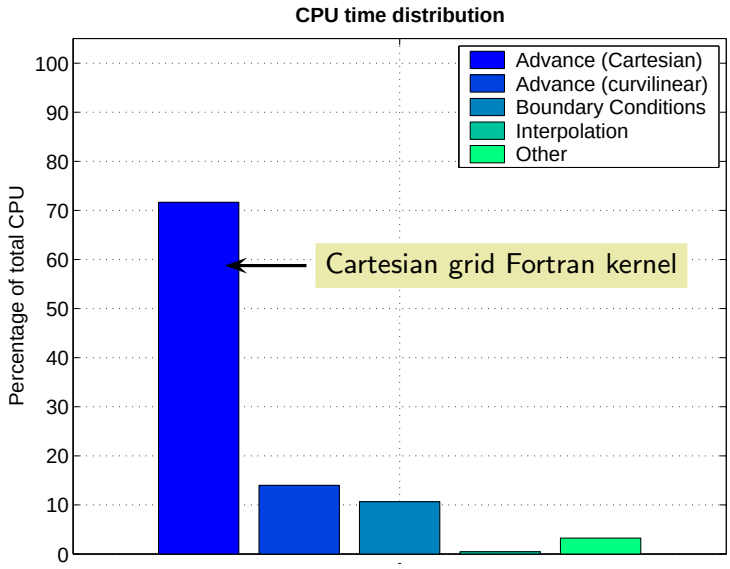
## A Parallel 4th-order accurate solver for the time-dependent Maxwell equations



Scattering of a plane wave by a cylinder. Top: scattered field $E_x$, $E_y$ and $H_z$ for $ka = 1/2$.
Bottom: scattered field $E_x$, $E_y$ and $H_z$ for $ka = 5/2$

14

**Performance of overlapping grid codes can approach that of Cartesian grid codes.**



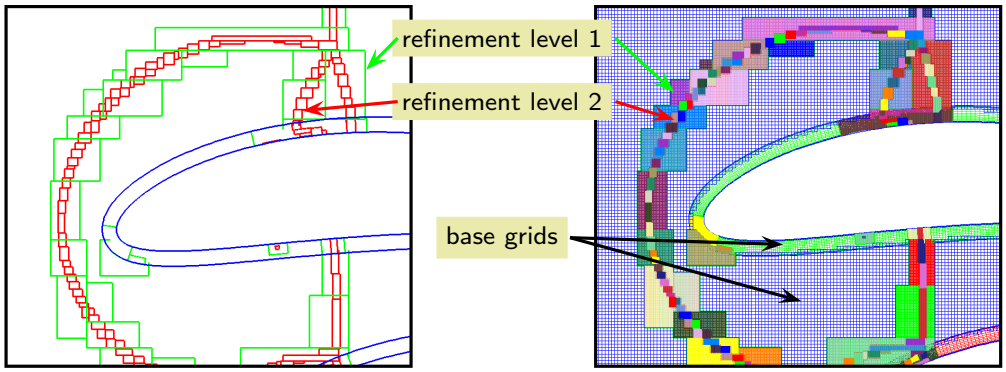

**Performance of the Maxwell solver (serial).**

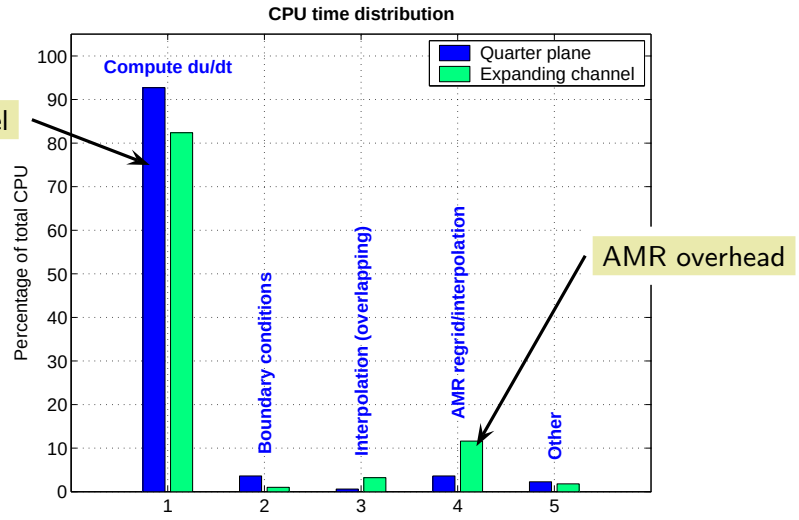
Two-dimensions, 3.8 million grid-points.



## Block Structured Adaptive Mesh Refinement and Overlapping Grids

- ♢ Refinement patches are generated in the parameter space of each component grid (base grid).
- ♢ Refinement patches are organized in a hierarchy of *refinement levels*.
- ♢ Error estimators determine where refinement is needed.
- ♢ AMR grid generation (Berger-Rigoutsos algorithm) builds refinement patches based on the error estimate.
- ♢ refinement grids may interpolate from refinement grids of different base grids.
- ♢ The key issue is efficiency.





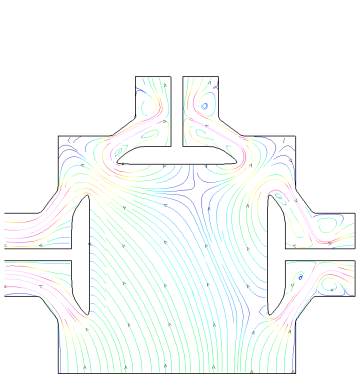

| | Quarter plane | Expanding channel |
|---|---|---|
| time steps | 12418 | 21030 |
| seconds per step | 14.94 | 13.96 |
| grids (min,ave,max) | $(2, 57, 353)$ | $(5, 274, 588)$ |
| points (min,ave,max) | $(2.0e5, 9.2e5, 1.9e6)$ | $(1.2e5, 6.4e5, 1.3e6)$ |

**Overlapping grid AMR performance on two detonation problems.**

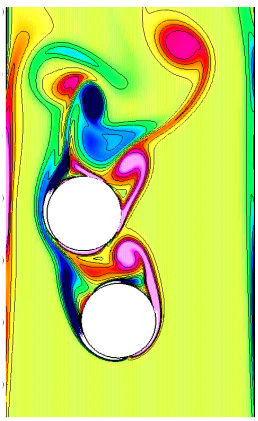


## Moving Overlapping Grids

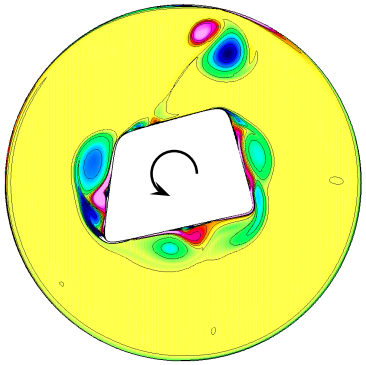
- ♢ Boundary fitted component grids are used to discretize each moving body.
- ♢ Grids move at each time step according to some governing equations.
- ♢ Overlapping connectivity information is updated by Ogen (interpolation points, discretization points, unused points).
- ♢ Solution values at **exposed points** are interpolated at previous time levels.
- ♢ Issue: Detection and treatment of collisions – elastic/in-elastic collisions
- ♢ Issue: Bodies that get very close – how should the grids interpolate



Moving valves (INS)

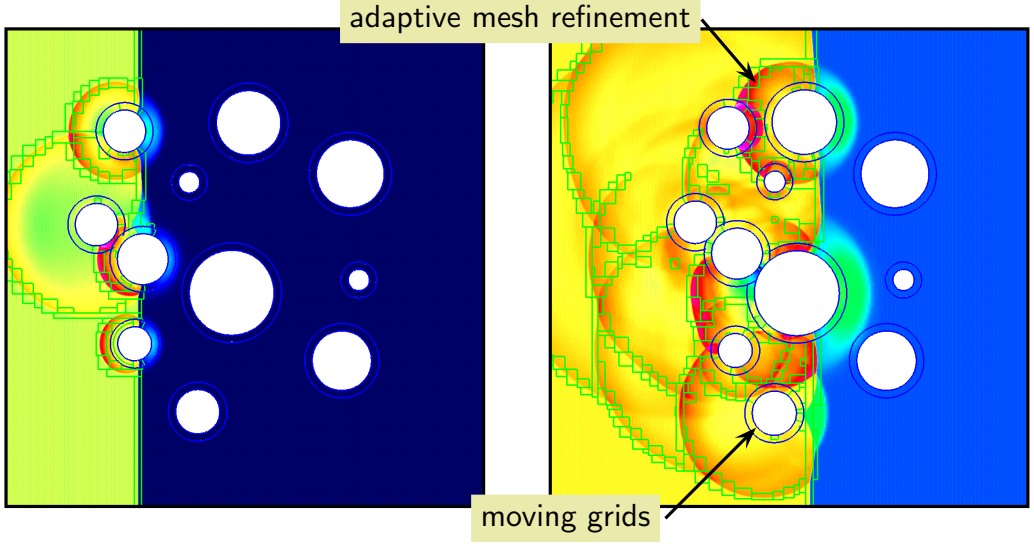


Falling cylinders (INS)



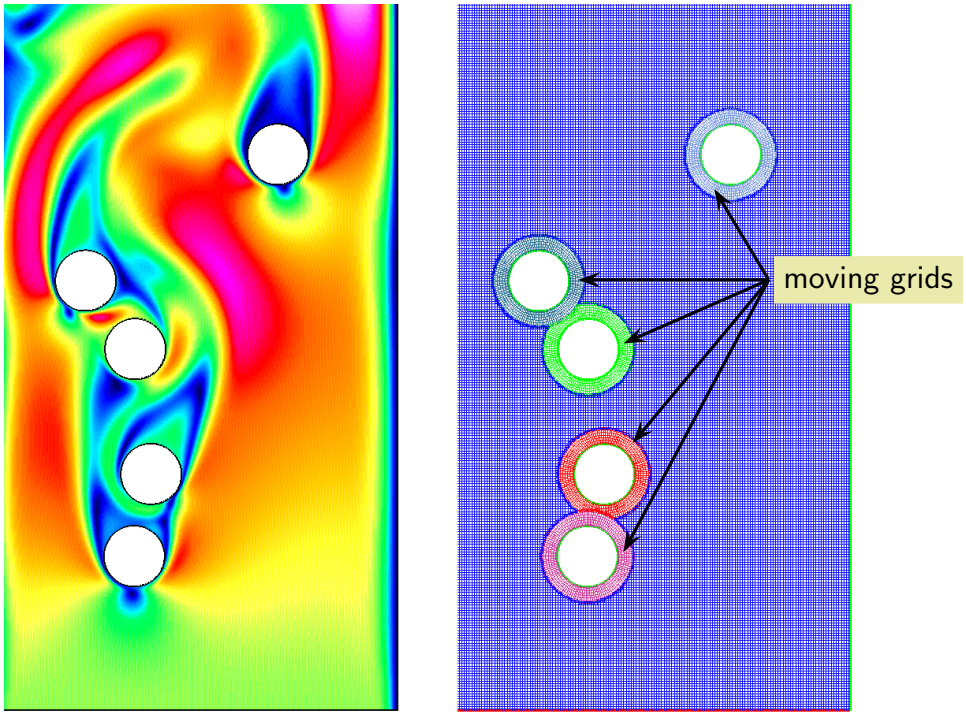
Rotating body (INS)

## Moving geometry and AMR



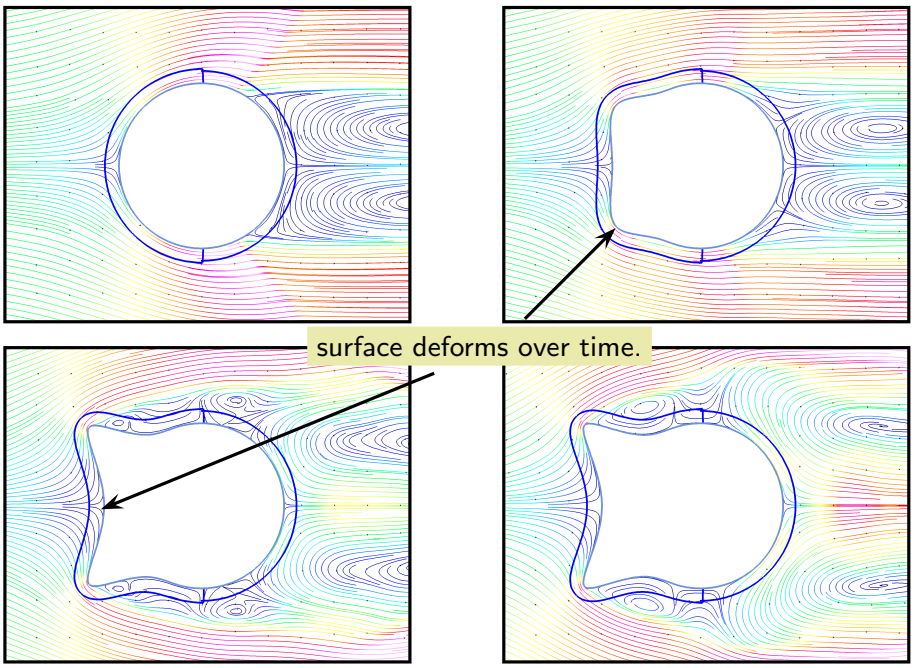

**A shock hitting a collection of cylinders (density).**






**Falling cylinders in an incompressible flow**

## Modeling Deforming Geometry with Overlapping Grids



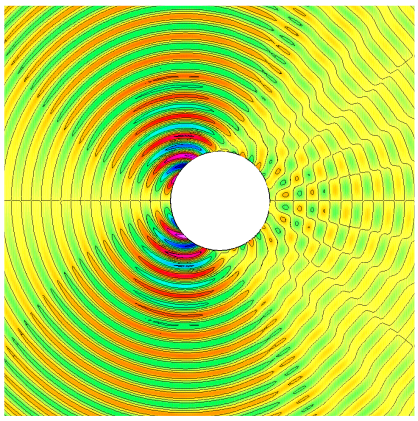

Streamlines of a compressible flow around a deforming boundary.

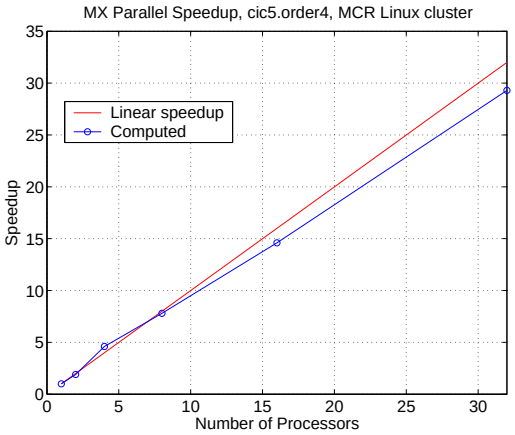


## The model for distributed parallel computing in Overture

- ♢ Grids can be distributed across one or more processors.
- ♢ Distributed parallel arrays using P++ (K. Brislawn, B. Miller, D. Quinlan)
- ♢ P++ uses Multiblock PARTI (A. Sussman, G. Agrawal, J. Saltz) for block structured communication with MPI (ghost boundary updates, copies between different distributed arrays)
- ♢ A special parallel overlapping grid interpolation routine is used for overlapping grid interpolation.

## Parallel scaling of the Maxwell solver – preliminary results





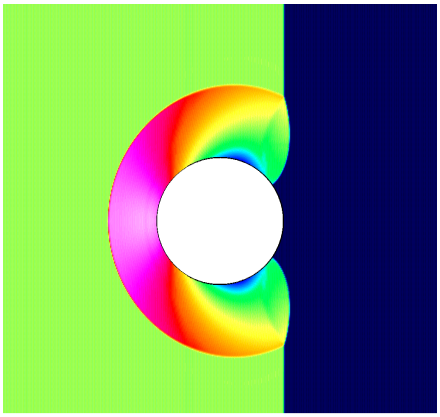

Fourth-order accurate

2D scattering from a cylinder

Fixed size problem, 3.8 million grid-points



## Euler equations: preliminary parallel results



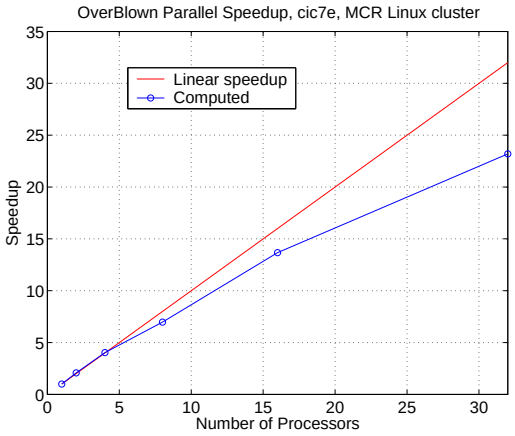
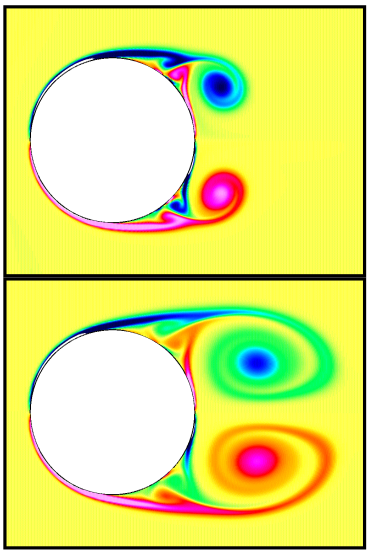



Figure 1: Left: the computation of a shock hitting a cylinder (density). Right: parallel speedup for this problem, keeping the problem size fixed (4 Million grid points), on a linux cluster (Xeon processors).

## Incompressible Navier-Stokes: preliminary parallel results



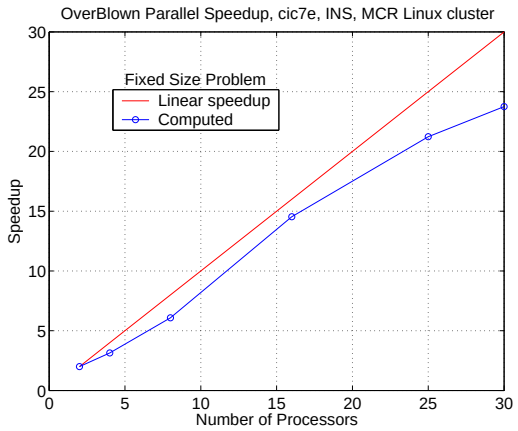



Figure 2: Left: impulsively started cylinder in an incompressible flow (vorticity). Right: parallel speedup keeping the problem size fixed (4 Million grid points), on a linux cluster (Xeon processors). The pressure equation is solved with algebraic multigrid (Hypre).